

CERTIFICATE

It is certified that the work contained in the thesis titled " *Heterocyclic Compounds as Corrosion Inhibitors for Mild Steel in Hydrochloric Acid Solution*" by "*Chandrabhan Verma*" has been carried out under my supervision and that this work has not been submitted elsewhere for a degree. It is further certified that the student has fulfilled all the requirements of Comprehensive Examination, Candidacy and SOTA for the award of Ph.D. Degree.

Prof. M.A. Quraishi

(Supervisor)

Department of Chemistry

Indian Institute of Technology,

Banaras Hindu University, Varanasi

221005

DECLARATION BY THE CANDIDATE

I, "*Chandrabhan Verma*", certify that the work embodied in this thesis is my own bona fide work and carried out by me under the supervision of "Prof. *M.A. Quraishi*" from "July-2012" to "Sept-2016", at the "*Department of Chemistry*", Indian Institute of Technology (BHU), Varanasi. The matter embodied in this thesis has not been submitted for the award of any other degree/diploma. I declare that I have faithfully acknowledged and given credits to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not willfully copied any other's work, paragraphs, text, data, results, etc., reported in journals, books, magazines, reports dissertations, theses, etc., or available at websites and have not included them in this thesis and have not cited as my own work.

Date :

Signature of the Student

Place:

Chandrabhan Verma

CERTIFICATE BY THE SUPERVISOR

It is certified that the above statement made by the student is correct to the best of my/our knowledge.

Prof. M.A. Quraishi

(Supervisor)

Department of Chemistry

Indian Institute of Technology,

Banaras Hindu University, Varanasi

221005

Prof. R.B. Rastogi

(Head)

Department of Chemistry

Indian Institute of Technology,

Banaras Hindu University, Varanasi

221005

COPYRIGHT TRANSFER CERTIFICATE

Title of the Thesis: *Heterocyclic Compounds as Corrosion Inhibitors for Mild Steel in Hydrochloric Acid Solution.*

Name of the Student: *Chandrabhan Verma*

Copyright Transfer The undersigned hereby assigns to the Institute of Technology (Banaras Hindu University) Varanasi all rights under copyright that may exist in and for the above thesis submitted for the award of the "*Doctor of Philosophy*".

Date :

Signature of the Student

Place:

Chandrabhan Verma

Note: However, the author may reproduce or authorize others to reproduce material extracted verbatim from the thesis or derivative of the thesis for author's personal use provided that the source and the Institute's copyright notice are indicated.

ACKNOWLEDGEMENTS

This thesis, the conclusion of several years' work, is a result that I could not have achieved without the support of many peoples to whom I would like to express my gratitude.

Foremost I would like to express my gratitude towards my supervisor Prof. M. A. Quraishi, Department of Chemistry, Indian Institute of Technology, Banaras Hindu University, Varanasi, for his constant guidance, valuable suggestions and kind encouragement during my association with his research group. I am thankful to Prof. (Mrs.) R. B. Rastogi, Head, Department of Chemistry, Indian Institute of technology, Banaras Hindu University, Varanasi. for providing necessary facilities during my research work.

My special thanks to all my RPC members, Prof. S. H. Hasan, Department of Chemistry, Indian Institute of Technology, Banaras Hindu University, Varanasi and Prof. Om Prakash Department of Ceramic Engineering , Indian Institute of Technology, Banaras Hindu University, Varanasi for their constant guidance, valuable suggestions and kind encouragement during my research work.

I am gratefully acknowledging the facilities provided by the Department of Metallurgical Engineering, Indian Institute of technology, Banaras Hindu University, Varanasi.

I have deep sense of gratitude for all Teachers of the Department of Chemistry, Indian Institute of technology, Banaras Hindu University, Varanasi for their cooperation and inspiration.

I am obliged to all my seniors and friends; Dr. Ishtiaque Ahamad, Dr. Deelip Kumar Yadav, Dr. Sudheer, Dr. Chitrasen Gupta, Dr. Ambrish Singh, Dr. Dheeraj Singh Chauhan, Mr. Kashif Rahmani Ansari, Mrs. Priyanka Singh, Md. Javed and Parvez Akhtar, Kritika Srivastava and Jiyaul Haque for their vital contributions in my research work.

I would like to acknowledge my indebtedness to my parents Mr. Somaroo Patel & Mrs. Chirauji Devi and my family member's for their love, affection, prayer and support.

I am thankful to non-teaching staff of Department of Chemistry, Indian Institute of technology, Banaras Hindu University, Varanasi.

I am also thankful to MHRD for providing financial assistance during my research work.

(Chandrabhan Verma)

Department of Chemistry

Indian Institute of Technology

(Banaras Hindu University)

Varanasi-221 005, India

TABLE OF CONTENTS

CHAPTER 1 INTRODUCTION	1-68
1.1.General Introduction	1
1.2.Types of corrosion	2
1.3.Forms of corrosion	6
1.4.Basic concept of corrosion	11
1.5. Factors influencing metallic corrosion	12
1.6.Corrosion thermodynamics	17
1.7.Kinetics of corrosion	23
1.8.Corrosion protection methods	28
1.9.Mechanism of corrosion inhibition in acid solution	35
1.10. Adsorptive Mechanism of corrosion inhibition	36
1.11. Inhibition of mild steel corrosion in minerals acids	42
1.12. Graphical representation of kinetic data	43
1.13. Electrochemical Impedance Spectroscopy (EIS)	49
1.14. Application of Theoretical Methods in Corrosion Inhibition Studies	52
1.15. Heterocyclic compounds as corrosion inhibitors: literature survey with particular emphasis of quantum chemical calculations and molecular dynamics simulations	58
CHAPTER 2: EXPERIEMNTAL	69-85
2.1. Materials	69
2.2. Heterocyclics inhibitors	70
2.3. Instruments and techniques	78

2.4. Determination of Thermodynamic Parameters	81
2.5. SEM, EDX and AFM measurements	82
2.6. Computational studies	83
CHAPTER 3: RESULTS AND DISCUSSIONS	86-177
3.1. 5-arylpyrimido-[4, 5-b] quinoline-diones (APQDs) as corrosion inhibitors	86
3.2. 2-amino-4-arylquinoline-3-carbonitriles (AACs) as corrosion inhibitors	111
3.3. 2, 4-diamino-5-(phenylthio)-5H-chromeno [2, 3-b] pyridine-3-carbonitriles (DHPCs) as corrosion inhibitors	132
3.4. 3-amino alkylated indoles (AAIs) as corrosion inhibitors	156
CHAPTER 4: SUMMARY	178-184
4.1. Summary	178
4.2. Conclusions	184
REFERENCES	185-213
LIST OF PUBLICATIONS	214-218

LIST OF FIGURES

Figure 1.1: liquid metal corrosion of mild steel surface by molten Copper at 1100 ⁰ C (MP: 1085 ⁰ C)	4
Figure 1.2: E-pH diagram for a generic metal M which forms hydroxides	20
Figure 1.3: Pourbaix diagram for iron/water system at 298 K	22
Figure 1.4: Schematic representation of Evans diagram for iron in acid solution	43
Figure 1.5: (a) Anodic control (b) cathodic control, (c) mixed control of a corrosion process.	44
Figure 1.6: Anodic and cathodic half-cell reactions present simultaneously on a corroding zinc surface	45
Figure 1.7: Polarization of anodic and cathodic half-cell reactions for zinc in acid solution to give a mixed potential, E_{corr} and a corrosion rate (current density)	46
Figure 1.8: “ E vs. i ” for Fe in acid solution	47
Figure 1.9: Extrapolated Tafel curves	48
Figure 1.10: Complex plane impedance spectrum	50
Figure 1.11: Nyquist plot along with constant phase element	50
Figure 3.1.1: (a) Arrhenius plots for the corrosion of mild steel in 1 M HCl (b) Langmuir adsorption isotherm plots for the adsorption of APQDs on mild steel surface in 1M HCl	92
Figure 3.1.2: Polarization curves for mild in absence and presence of different concentrations APQDs	95

Figure 3.1.3: Nyquist curves for mild in absence and presence of different concentrations of APQDs 97

Figure 3.1.4: Bode impedance modulus ($\log f$ vs $\log |Z|$) and phase angle ($\log f$ vs α^0) plots for mild steel in 1 M HCl in absence and different of different concentrations of (a) APQD-1, (b) APQD-2, (c) APQD-3 and (d) APQD-4. 99

Figure 3.1.5: SEM images of mild steel surfaces: abraded (a), in 1 M HCl in the absence of APQDs (b), and in 1 M HCl in the presence of 20 mgL⁻¹ of APQD-1 (c), APQD-2 (d), APQD-3 (e) and APQD-4 (f) 101

Figure 3.1.6: AFM images of mild steel: (a) in absence of APQDs and in the presence of 20 mgL⁻¹ of (b) APQD-1, (c) APQD-2, and (d) APQD-3 (e) APQD-4 102

Figure 3.1.7: Optimized molecular structures of (a) APQD-1, (b) APQD-2, (c) APQD-3 and (d) APQD-4 103

Figure 3.1.8: The frontier molecular orbital (left-hand side: HOMO; and right-hand side: LUMO) of the studied APQDs (a) APQD-1 (b) APQD-2, (c) APQD-3, and (d) APQD-4 105

Figure 3.1.9: Fukui indices for the electrophilic (f_k^+) and nucleophilic (f_k^-) sites for (a) APQD-1, (b) APQD-2, (c) APQD-3, and (d) APQD-4. (All the surfaces were visualized at isosurface value of 0.004, except for the f_k^+ of (c) APQD-3, and (d) APQD-4 for which isosurface value of 0.0028 and 0.0025 respectively, were used for better visualization) 108

Figure 3.1.10: Side view equilibrium adsorption of APQD-1, APQD-2, APQD-3 and APQD-4 on Fe (110) surface (a) before and (b) after molecular dynamics simulations

Figure 3.2.1: (a) Variation of inhibition efficiency with AACs concentration (b) Arrhenius plots of $\log C_R$ vs. $1000/T$ (c) Langmuir isotherm plot for the adsorption of the AACs on mild steel surface in 1M HCl	115
Figure 3.2.2: Polarization curves for mild in absence and presence of different concentration of AACs	117
Figure 3.2.3: Nyquist plot for mild steel in 1 M HCl without and with different concentrations of AACs	120
Figure 3.2.4: Bode ($\log f$ vs $\log Z $) and phase angle ($\log f$ vs α^0) plots for mild steel in 1 M HCl in absence and presence of different concentration of AACs	122
Figure 3.2.5: SEM images of mild steel surfaces: abraded (a), in absence of AACs (b) in the presence of 40 mgL^{-1} of AAC-1(c), AAC-2(d), and AAC-3(e)	123
Figure 3.2.6: EDX images of mild steel: (a) in absence of AACs and in the presence of 40 mgL^{-1} of (b) AAC-1, (c) AAC-2, and (d) AAC-3	125
Figure 3.2.7: AFM images of mild steel: (a) in absence of AACs and in the presence of 40 mgL^{-1} of (b) AAC-1, (c) AAC-2, and (d) AAC-3	126
Figure 3.2.8: Optimized molecular structures of the studied compounds showing the dihedral angles a-b-c-d (in degrees)	127
Figure 3.2.9: The frontier molecular orbital of studied AACs (a) AAC-1 (left, HOMO; right, LUMO), (b) AAC-2 (left, HOMO; right, LUMO) and (c) AAC-3 (left, HOMO; right, LUMO)	129
Figure 3.3.1: (a) Arrhenius plots for the corrosion of mild steel in 1 M HCl in the presence of the studied inhibitors (b) Langmuir adsorption isotherms for mild steel in 1 M	

Figure 3.3.2: Polarization curves recorded for mild steel in the absence and presence of different concentrations DHPCs 139

Figure 3.3.3: Nyquist plots recorded for mild steel in 1 M HCl in the absence and presence of different concentrations of (a) DHPC-1, (b) DHPC-2, and (c) DHPC-3 142

Figure 3.3.4: Bode impedance modulus ($\log f$ vs $\log |Z|$) and phase angle ($\log f$ vs α^0) plots for mild steel in 1 M HCl in the absence and presence of different of different concentrations of (a) DHPC-1, (b) DHPC-2, and (c) DHPC-3 144

Figure 3.3.5: SEM images of mild steel surfaces in 1 M HCl in the absence of DHPCs (a), and in 1 M HCl in the presence of optimum concentration of DHPC-1 (b), DHPC-2 and (c), DHPC-3 (d) 145

Figure 3.3.6: AFM images of mild steel surfaces in 1 M HCl in the absence of DHPCs (a), and in 1 M HCl containing optimum concentration of DHPC-1 (b)HPC-2 and (c), DHPC-3(d) 146

Figure 3.3.7: Optimized molecular structures of (a) DHPC-1, (b) DHPC-2, and (c) DHPC-3 148

Figure 3.3.8: The frontier molecular orbital (left-hand side: HOMO; and right-hand side: LUMO) of the studied DHPCs (a) DHPC-1 (b) DHPC-2, and (c) DHPC-3 . 149

Figure 3.3.9: Fukui indices f^+ and f^- corresponding to the atomics sites for the nucleophilic and electrophilic attacks respectively in (a) DHPC-1, (b) DHPC-2, and (c) DHPC-3 (*isosurface value = 0.003*) 152

Figure 3.3.10: Side and top views of the most stable adsorption models of (a) DHPC-1, (b) DHPC-2, and (c) DHPC-3 on Fe (110) surface using quench molecular dynamic	154
Figure 3.4.1: (a) Arrhenius plots of $\log C_R$ vs. $1000/T$ (b) Langmuir isotherm plot for the adsorption of the AAI's on mild steel surface in 1M HCl	161
Figure 3.4.2: Polarization curves recorded for mild steel in the absence and presence of different concentrations of AAI's	163
Figure 3.4.3: Nyquist plots recorded for mild steel in 1 M HCl in the absence and presence of different concentrations of AAI's.	165
Figure 3.4.4: Bode impedance modulus ($\log f$ vs $\log Z $) and phase angle ($\log f$ vs α^0) plots for mild steel in 1 M HCl in the absence and different of different concentrations of AAI's	168
Figure 3.4.5: SEM images of mild steel surfaces in 1 M HCl in the absence of AAI's (a), and in 1 M HCl in the presence of optimum concentration of AAI-1 (b), AAI-2 and (c), AAI-3(d)	169
Figure 3.4.6: AFM images of mild steel surfaces in 1 M HCl in the absence of AAI's (a), and in 1 M HCl in the containing optimum concentration of AAI-1 (b), AAI-2 and (c), AAI-3(d)	170
Figure 3.4.7: Optimized molecular structures of studied AAI's, (a) AAI-1, (b) AAI-2 and (c) AAI-3	172
Figure 3.4.8: The frontier molecular orbital (left-hand side: HOMO; and right-hand side: LUMO) of the studied APQDs (a) AAI-1 (b) AAI-2 and (c) AAI-3	173

Figure 3.4.9: Side view equilibrium adsorption of AAI-1, AAI-2, and AAI-3 on Fe (110) surface
(left hand side: before; and right hand side: after molecular dynamics simulations)

LIST OF TABLES

Table 1.1: ASM classifications of corrosion types	8
Table 1.2: Different adsorption isotherms	38
Table 2.1: IUPAC name, molecular structure, molecular formula, melting point and analytical data of studied APQDs	72
Table 2.2: IUPAC name, molecular structure, molecular formula, melting point and analytical data of studied AACs	74
Table 2.3: IUPAC name, molecular structure, molecular formula, melting point and analytical data of the studied DHPCs	76
Table 2.4: IUPAC name, molecular structure, molecular formula, and analytical data of AAI	77
Table 3.1.1: IUPAC name, molecular structure and abbreviation of the studied APQDs	88
Table 3.1.2: The weight loss parameters obtained for mild steel in 1 M HCl containing different concentrations of APQDs	89
Table 3.1.3: Variation of C_R and η % with temperature in absence and presence of optimum concentration of APQDs in 1M HCl	90
Table 3.1.4: The values of K_{ads} and ΔG_{ads}° for mild steel in absence and presence of optimum concentration of APQDs in 1M HCl at different studied temperature	93
Table 3.1.5: Tafel polarization parameters for mild steel in 1 M HCl solution in absence and presence of different concentrations of APQDs	96
Table 3.1.6: EIS parameters obtained for mild steel in 1 M HCl in absence and presence of different concentrations of APQDs	98

Table 3.1.7: Quantum chemical parameters derived from the B3LYP/6-31+G(d,p) method	106
Table 3.1.8: Interaction energies between the inhibitors and Fe (110) surface (in kJmol^{-1})	108
Table 3.2.1: IUPAC name, molecular structure, and abbreviation of the studies inhibitors	112
Table 3.2.2: The weight loss parameters obtained for mild steel in 1 M HCl containing different concentrations of AACs	113
Table 3.2.3: Variation of C_R and η % with temperature in absence and presence of optimum concentration of AACs in 1M HCl	114
Table 3.2.4: The values of K_{ads} and $\Delta G^{\circ}_{\text{ads}}$ for mild steel in absence and presence of optimum concentration of AACs in 1M HCl at different studied temperature	116
Table 3.2.5: Tafel polarization parameters for mild steel in 1 M HCl solution in absence and at different concentrations of AACs	118
Table 3.2.6: EIS parameters obtained for mild steel in 1 M HCl in absence and presence of different concentration of AACs	121
Table 3.2.7: Percentage atomic contents of elements obtained from EDX spectra for AACs	125
Table 3.2.8: Quantum chemical parameters derived from the B3LYP/6-31+G(d,p) method	131
Table 3.3.1: IUPAC names, molecular structures, and abbreviations of the studied DHPCs	134
Table 3.3.2: The weight loss parameters obtained for mild steel in 1 M HCl containing different concentrations of DHPCs	135
Table 3.3.3: Variation of C_R and η % with temperature in the absence and presence of optimum concentration of DHPCs in 1M HCl	136
Table 3.3.4: The values of K_{ads} and $\Delta G^{\circ}_{\text{ads}}$ for mild steel in 1 M HCl in the absence and presence of optimum concentration of DHPCs at different temperatures.	138

Table 3.3.5: Tafel polarization parameters for mild steel in 1 M HCl solution in the absence and presence of different concentrations of DHPCs	140
Table 3.3.6: EIS parameters obtained for mild steel in 1 M HCl in the absence and presence of different concentrations of DHPCs	143
Table 3.3.7: Some relevant quantum chemical parameters of the studied compounds	151
Table 3.3.8: Interaction energies between the inhibitors and Fe (110) surface (kcal/mol)	155
Table 3.4.1: IUPAC names, molecular structures, and abbreviations data of studied AAI	158
Table 3.4.2: The weight loss parameters obtained for mild steel in 1 M HCl containing different concentrations of AAI	159
Table 3.4.3: Variation of C_R and η % with temperature in absence and presence of optimum concentration of AAI in 1M HCl	.160
Table 3.4.4: The values of K_{ads} and ΔG°_{ads} for mild steel in absence and presence of optimum concentration of AAI in 1M HCl at different studied temperature	162
Table 3.4.5: Tafel polarization parameters for mild steel in 1 M HCl solution in absence and presence of different concentrations of AAI	164
Table 3.4.6: EIS parameters obtained for mild steel in 1 M HCl in absence and presence of different concentrations of AAI	166
Table 3.4.7: Quantum chemical parameters derived from the B3LYP/6-31+G(d,p) method.	
Table 3.4.8: Interaction energies between the inhibitors and Fe (110) surface (Kcal/mol)	174

ABBREVIATIONS USED

$\eta\%$ = Percentage of inhibition efficiency

C_R = Corrosion rate ($\text{mgcm}^{-2}\text{h}^{-1}$)

C_R^o = Corrosion rate in uninhibited system ($\text{mgcm}^{-2}\text{h}^{-1}$)

C_R^i = Corrosion rate in inhibited system ($\text{mgcm}^{-2}\text{h}^{-1}$)

E.W. = Equivalent weight of mild steel

D = Density of metal (g cm^{-3})

Q = magnitude of the CPE ($\Omega^{-1} \text{s}^n \text{cm}^{-2}$)

j = imaginary unit ($\sqrt{-1}$)

ω = angular frequency ($2\pi f$, f the frequency)

f = Frequency of component of impedance (s^{-1})

C_{dl} = Double layer capacitance ($\mu\text{F cm}^{-2}$)

R_s = Solution resistance (Ωcm^2)

R_t^o = charge transfer resistance in absence of inhibitor (Ωcm^2)

R_t^i = charge transfer resistance in presence of inhibitor (Ωcm^2)

I_{corr}^o = Corrosion current density in uninhibited solution (mA cm^{-2})

I_{corr}^i = Corrosion current density in inhibited solution (mA cm^{-2})

E_{corr} = Corrosion potential (mV/SCE)

β_a = Anodic Tafel constant (mVdec^{-1})

β_c = Cathodic Tafel constant (mVdec^{-1})

λ = Arrhenius pre-exponential factor ($\text{mg cm}^{-2} \text{h}^{-1}$)

E_a = Activation energy (kJ mol^{-1})

R = Universal gas constant ($\text{J K}^{-1} \text{mol}^{-1}$)

T = Absolute temperature (K)

N = Avogadro's number ($6.023 \times 10^{23} \text{mol}^{-1}$)

h = Planck's constant (J-s)

K_{ads} = Adsorption equilibrium constant (M^{-1})

$\Delta G^\circ_{\text{ads}}$ = Gibbs free energy of adsorption (kJ mol^{-1})

θ = Degree of surface coverage of metal

C_{inh} = Concentration of inhibitor (mol L^{-1} , ppm)

E_{HOMO} = Energy of highest occupied molecular orbital

E_{LUMO} = Energy of lowest unoccupied molecular orbital

$\Delta E_{\text{L-H}}$ = Energy gap between HOMO and LUMO

ΔN = Number of electron transferred

ΔE_{MBG} = Singlet-triplet molecular band gap

χ_{Fe} = Electronegativity of iron

χ_{inh} = Electronegativity of inhibitor

η_{Fe} = Hardness of iron

η_{inh} = Hardness of inhibitor

ΔN = Fraction of electron transfer

IP = Vertical ionization potential of inhibitor

EA = Vertical electron affinity of inhibitor

ΔE_{T} = Total energy transfer after inhibitor adsorption

E_{total} = Sum of energies of inhibitor molecule and metallic surface

$E_{\text{Fe surface}}$ = Energy of metallic surface before inhibitor adsorption

E_{molecule} = Energy of the inhibitor molecule before adsorption of inhibitor molecules

$E_{\text{interaction}}$ = Interaction energy between metal surface and inhibitor molecules

E_{ads} = Adsorption energy.

PREFACE

Corrosion is a phenomenon of universal interest; it is degradation of materials particularly metals and alloys by electrochemical interaction with the environment. Corrosion can be very expensive as well as unsafe due to failures of various kinds and the need for expensive replacements which may occur even though the amount of metal destroyed is quite small. Due to increased use of metals and alloys in all fields of science and technology and increased pollution of air and water which generates more corrosive environments, the knowledge of corrosion and its prevention has become necessary. The annual global cost of corrosion was estimated to be around \$ US 2.5 trillion which constitute about 3% of the world GDP. However, the cost of corrosion can be reduced about 20-25% by applying recently available methods of corrosion prevention. Nowadays, the corrosion inhibitors is being used as the most popular and effective technique for combating corrosion. As the title itself reflects, the thesis highlights the attempts made in developing heterocyclic compounds such as 5-arylpyrimido-[4, 5-b] quinoline-diones, 2-amino-4-arylquinoline-3-carbonitriles, 2, 4-diamino-5-(phenylthio)-5H-chromeno [2, 3-b] pyridine-3-carbonitriles and 3-amino alkylated indoles as corrosion inhibitors.

The thesis starts with introduction highlighting the technological and economic significance of the problems associated with corrosion. The various forms and theories of corrosion have been described in order to explain the mechanism of corrosion. In the later part of the introduction, different measures of metallic corrosion inhibition with particular emphasis of heterocyclic compounds as corrosion inhibitors in acid solution have been described. The literature on the metallic corrosion inhibition by heterocyclic compounds as corrosion inhibitors

has been surveyed. The results obtained from the gravimetric and electrochemical techniques have been discussed section wise in terms of several commonly used corrosion parameters such as percentage inhibition efficiency ($\eta\%$), corrosion rate (C_R), charge transfer resistance (R_{ct}), corrosion current (i_{corr}) and corrosion potential (E_{corr}). The activation and thermodynamic parameters have also been calculated in order to find mechanistic information about the adsorption of inhibitor molecules on the metallic surface. The effects of inhibitors concentration and solution temperature on inhibition efficiency of the heterocyclic compounds have also been discussed. The SEM, EDX and AFM studies have been employed to confirm the presence of protective film of inhibitors on the mild steel surface. The DFT based quantum chemical calculations and molecular dynamics simulations have been carried out in order to correlate experimentally determined inhibition efficiencies with several computed parameters such as energy of highest occupied and lowest unoccupied molecular orbitals, E_{HOMO} and E_{LUMO} , respectively, energy band gap (ΔE), global hardness (η) and softness (ρ), electronegativity (χ), fraction of electron transfer (ΔN) and dipole moment (μ). A possible mechanism of corrosion has been proposed on the basis of experimental and computational analysis.

Major part of the thesis has been published in *RSC Advances* 6 (2016) 15639-15654, *RSC Advances* 5 (104), 85417-85430, *RSC Advances* 6 (2016) 53933-53948, and *Journal of Molecular Liquids* 219 (2016) 647-660.